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Calculating the influence of substituents upon the dissociation constants of carboxylic acids

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Abstract

1. A general formula was proposed for calculating the dissociation constants of substituted acids, considering all the electrostatic interactions in dissociated and nondissociated forms of substituted and unsubstituted acids. 2. Interactions of the charge- induced dipole type play an important role in a number of cases, in particular, determining the ortho- effect to one degree or another. 3. The values of ΔpK were calculated for ortho-toluic and propionic acids in accord with the experimental data. © 1968 Consultants Bureau.

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